

Transverse spin gradient functional for non-collinear spin density functional theory

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We present a novel functional for spin density functional theory aiming at the description of non-collinear magnetic structures. The construction of the functional employs the spin-spiral-wave state of the uniform electron gas as reference system. We show that the functional depends on transverse gradients of the spin magnetization, i.e., that in contrast to the widely used local spin density approximation the functional is sensitive to local changes of the direction of the spin magnetization. As a consequence the exchange-correlation magnetic field is not parallel to the spin magnetization and a local spin-torque is present in the ground state of the Kohn-Sham system. As a proof-of-principle we apply the functional to a Chromium mono-layer in the non-collinear 120°-Néel state.

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Density functional theory (DFT) [1] is presently the most widely used approach to determine the electronic structure of atoms, molecules and solids. Shortly after the original formulation by Hohenberg and Kohn [2] in terms of the electronic density $n(\mathbf{r})$ the theory was extended to include also the spin magnetization $\mathbf{m}(\mathbf{r})$ as fundamental variable [3]. Spin density functional theory (SDFT) applies to Hamiltonians of the form

$$\hat{\mathcal{H}} = \hat{\mathcal{T}} + \hat{\mathcal{V}} + \hat{\mathcal{B}} + \hat{\mathcal{W}}, \quad (1)$$

where in addition to the kinetic energy $\hat{\mathcal{T}}$, the potential energy $\hat{\mathcal{V}}$ and the electron-electron interaction energy $\hat{\mathcal{W}}$ (usually the Coulomb repulsion between two electrons) an additional energy contribution $\hat{\mathcal{B}}$ due to an external magnetic field $\mathbf{B}(\mathbf{r})$ is considered, i.e.,

$$\hat{\mathcal{B}} = -\mu_B \int d^3r \mathbf{B}(\mathbf{r}) \cdot \hat{\mathbf{m}}(\mathbf{r}). \quad (2)$$

The operator $\hat{\mathbf{m}}(\mathbf{r}) = \hat{\Phi}^\dagger(\mathbf{r}) \boldsymbol{\sigma} \hat{\Phi}(\mathbf{r})$, representing the spin magnetization, is defined in terms of the spinor field $\hat{\Phi}^\dagger(\mathbf{r}) = (\hat{\phi}_\uparrow^\dagger(\mathbf{r}) \hat{\phi}_\downarrow^\dagger(\mathbf{r}))$ and the vector of Pauli matrices $\boldsymbol{\sigma}$. As always in DFTs the success of the theory hinges on the availability of accurate and physically sound approximations to the exchange-correlation (xc) energy $E_{xc}[n, \mathbf{m}]$ - a functional of $n(\mathbf{r})$ and $\mathbf{m}(\mathbf{r})$ in the case of SDFT.

A straight-forward extension of the local density approximation (LDA) [4] to SDFT yields

$$E_{xc}^{\text{LSDA}}[n, \mathbf{m}] = \int d^3r n(\mathbf{r}) \varepsilon_{xc}^{\text{unif}}(n(\mathbf{r}), m(\mathbf{r})), \quad (3)$$

the so-called local spin density approximation (LSDA), with $m(\mathbf{r})$ being the magnitude of $\mathbf{m}(\mathbf{r})$ and $\varepsilon_{xc}^{\text{unif}}$ the xc energy of a spin-polarized uniform electron gas (UEG). For collinear magnetism, i.e., $\mathbf{m}(\mathbf{r})$ pointing in the same

direction everywhere in space, a plethora of functionals was derived (cf. Ref. 5) improving over the *collinear* LSDA, however, much less is known about constructing functionals for *non-collinear* magnetism, where the direction of $\mathbf{m}(\mathbf{r})$ is allowed to vary freely in space. In fact, most applications of non-collinear SDFT up-to-date are based on the idea, pioneered by Kübler et al. [6], to apply collinear functionals to non-collinear systems by evaluating the functional in a *local* reference frame with the local z -axis determined by the direction of $\mathbf{m}(\mathbf{r})$. The LSDA, defined in Eq. (3), employs a local reference frame intrinsically, which can be seen by evaluating the corresponding xc magnetic field

$$\mathbf{B}_{xc}^{\text{LSDA}}(\mathbf{r}) = -\frac{\delta E_{xc}^{\text{LSDA}}[n, \mathbf{m}]}{\delta \mu_B \mathbf{m}(\mathbf{r})} = -\frac{\partial \varepsilon_{xc}^{\text{unif}}}{\partial m} \frac{n(\mathbf{r}) \mathbf{m}(\mathbf{r})}{\mu_B m(\mathbf{r})}. \quad (4)$$

By construction $\mathbf{B}_{xc}^{\text{LSDA}}$ is always aligned with \mathbf{m} . The same is true for generalized gradient approximations (GGAs) employing the aforementioned rotation to a local reference frame. In recent years attempts were made to extend GGAs and meta-GGAs to non-collinear systems without invoking a local reference frame in order to produce a $\mathbf{B}_{xc}(\mathbf{r})$ which is non-collinear w.r.t. $\mathbf{m}(\mathbf{r})$ [7]. Since collinear functionals are usually formulated in terms of $n_\uparrow(\mathbf{r})$ and $n_\downarrow(\mathbf{r})$ (as opposed to $n(\mathbf{r})$ and $m(\mathbf{r})$) and gradients thereof, these approaches require a prescription mapping the gradient of $\mathbf{m}(\mathbf{r})$ (which is a 3×3 -matrix for non-collinear systems) to gradients of $n_\uparrow(\mathbf{r})$ and $n_\downarrow(\mathbf{r})$. Yet another approach was to consider the variations of the direction of $\mathbf{m}(\mathbf{r})$ perturbatively [8, 9]. In this letter we show that the very idea of the LSDA can be extended in a non-perturbative way to yield a new functional for SDFT depending on transverse gradients.

In the LSDA the spin polarized UEG is chosen as reference system to determine the local xc energy. Note that the LSDA does not employ the ground-state xc energy of the UEG, but instead the minimal xc energy of the

UEG under the *constraint* that its spin magnetization is m_0 . The new functional is based on the idea to consider a reference system with a non-collinear spin magnetization. In close analogy to the LSDA the local xc energy is determined from the UEG constrained to be in the so-called spin-spiral-wave (SSW) state [10]. The SSW state of the UEG is characterized by a constant density n_0 and a spin magnetization of the form

$$\mathbf{m}_0(\mathbf{r}) = m_0 \begin{pmatrix} s \cos(\mathbf{q} \cdot \mathbf{r}) \\ s \sin(\mathbf{q} \cdot \mathbf{r}) \\ \sqrt{1 - s^2} \end{pmatrix}, \quad (5)$$

with $s = \sin(\theta)$ and θ is the azimuthal angle between the rotating part (in the x - y plane) and the constant part (parallel to z -axis). The xc energy of the SSW UEG depends on four parameters: n_0 , m_0 , s and $q = |\mathbf{q}|$. As we will see below it is possible to define *local* $s(\mathbf{r})$ and $q(\mathbf{r})$ in terms of transverse gradients of $\mathbf{m}(\mathbf{r})$ which leads to the definition of the SSW functional

$$E_{xc}^{\text{SSW}}[n, \mathbf{m}] = \int d^3r n(\mathbf{r}) \varepsilon_{xc}^{\text{SSW}}(n(\mathbf{r}), m(\mathbf{r}), s(\mathbf{r}), q(\mathbf{r})), \quad (6)$$

where $\varepsilon_{xc}^{\text{SSW}}$ is the minimal xc energy of the UEG under the *constraint* that it is in the SSW state specified by $n(\mathbf{r})$, $m(\mathbf{r})$, $s(\mathbf{r})$ and $q(\mathbf{r})$. It is important to realize that the LSDA is included in this definition in the limits $s \rightarrow 0$ or $q \rightarrow 0$, i.e., $\varepsilon_{xc}^{\text{SSW}}(n, m, s, q = 0) = \varepsilon_{xc}^{\text{SSW}}(n, m, s = 0, q) = \varepsilon_{xc}^{\text{SSW}}(n, m, s = 0, q = 0) = \varepsilon_{xc}^{\text{unif}}(n, m)$. This can be emphasized by rewriting the SSW functional as

$$E_{xc}^{\text{SSW}}[n, \mathbf{m}] = \int d^3r n(\mathbf{r}) \varepsilon_{xc}^{\text{unif}}(n(\mathbf{r}), m(\mathbf{r})) \times (1 + S_{xc}(n(\mathbf{r}), m(\mathbf{r}), s(\mathbf{r}), q(\mathbf{r}))), \quad (7)$$

where we introduced the spin gradient extension (SGE)

$$S_{xc}(n, m, s, q) = \frac{\varepsilon_{xc}^{\text{SSW}}(n, m, s, q) - \varepsilon_{xc}^{\text{unif}}(n, m)}{\varepsilon_{xc}^{\text{unif}}(n, m)}. \quad (8)$$

Before we discuss the explicit form of the local $s(\mathbf{r})$ and $q(\mathbf{r})$ we briefly discuss *global*, i.e., spatially independent, rotations of the internal (spin) space. These rotations correspond to transforming $\Phi(\mathbf{r}) \rightarrow \mathcal{U}\Phi(\mathbf{r})$, where \mathcal{U} is an element of $\text{SU}(2)$ (a rotation of the internal [spin] degree of freedom). Note that *spatial* vectors, e.g. the paramagnetic current $\mathbf{j}_p(\mathbf{r})$, are invariant under such internal rotations whereas *spin* vectors as $\mathbf{m}(\mathbf{r})$ transform as $\mathbf{m}(\mathbf{r}) \rightarrow \underline{R}\mathbf{m}(\mathbf{r})$, with \underline{R} being the 3×3 rotation matrix corresponding to \mathcal{U} . Since the kinetic energy \hat{T} and the interaction energy \hat{W} are invariant under global rotations of the internal space it follows that $E_{xc}[n, \mathbf{m}] = E_{xc}[n, \underline{R}\mathbf{m}]$. Considering infinitesimal spin rotations one obtains the so-called zero-torque theorem

$$0 = \int d^3r \mathbf{m}(\mathbf{r}) \times \mathbf{B}_{xc}(\mathbf{r}), \quad (9)$$

which was first derived by Capelle et al. [11] via the equation of motion for the spin magnetization. It states that \mathbf{B}_{xc} *cannot* exert a net torque on \mathbf{m} .

A simple rule to follow in order to ensure that explicit functionals for SDFT obey the zero-torque theorem is to write $E_{xc}[n, \mathbf{m}]$ in terms of proper scalars, i.e., spin indices have to be contracted with spin indices and spatial indices with spatial indices. This implies that the determination of the local xc energy in terms of *strictly* local densities is exhausted by $n(\mathbf{r})$ and $m(\mathbf{r})$. Hence the local $s(\mathbf{r})$ and $q(\mathbf{r})$ have to be determined from properly contracted gradients of $\mathbf{m}(\mathbf{r})$.

Let us first look at $D(\mathbf{r}) = |\nabla \otimes \mathbf{m}(\mathbf{r})|^2$, which corresponds to the *total* first order change of $\mathbf{m}(\mathbf{r})$. It can be split into a *longitudinal* contribution $D_L(\mathbf{r})$ and a *transverse* contribution $D_T(\mathbf{r})$, i.e.,

$$D(\mathbf{r}) = \frac{1}{m^2(\mathbf{r})} (D_L(\mathbf{r}) + D_T(\mathbf{r})), \quad (10)$$

$$D_L(\mathbf{r}) = |\mathbf{m}(\mathbf{r}) \cdot (\nabla \otimes \mathbf{m}(\mathbf{r}))|^2, \quad (11)$$

$$D_T(\mathbf{r}) = |\mathbf{m}(\mathbf{r}) \times (\nabla \otimes \mathbf{m}(\mathbf{r}))|^2, \quad (12)$$

where the meaning of longitudinal and transverse is defined by the local direction of $\mathbf{m}(\mathbf{r})$. For the SSW UEG the two contributions are $D_L^{\text{SSW}} = 0$ and $D_T^{\text{SSW}} = m_0^4 s^2 q^2$. Both contributions are constant in space for the SSW UEG and hence play a similar role as the density n_0 and the magnitude of the spin magnetization m_0 , i.e., they locally characterize the state. D_L^{SSW} vanishes because the spin magnetization in the SSW UEG only rotates. D_T does not vanish but it only determines the combination sq .

Accordingly we look at the second order variation $d(\mathbf{r}) = |\nabla^2 \mathbf{m}(\mathbf{r})|^2$. Again, it can be analyzed w.r.t. longitudinal and transverse contributions

$$d(\mathbf{r}) = \frac{1}{m^2(\mathbf{r})} (d_L(\mathbf{r}) + d_T(\mathbf{r})), \quad (13)$$

$$d_L(\mathbf{r}) = |\mathbf{m}(\mathbf{r}) \cdot (\nabla^2 \mathbf{m}(\mathbf{r}))|^2, \quad (14)$$

$$d_T(\mathbf{r}) = |\mathbf{m}(\mathbf{r}) \times (\nabla^2 \mathbf{m}(\mathbf{r}))|^2. \quad (15)$$

For our reference system this yields $d_L^{\text{SSW}} = m_0^4 s^4 q^4$ and $d_T^{\text{SSW}} = m_0^4 (1 - s^2) s^2 q^4$. The change of $\mathbf{m}(\mathbf{r})$ to first order is perpendicular to $\mathbf{m}(\mathbf{r})$, but to second order $\mathbf{m}(\mathbf{r})$ also changes in the direction of $\mathbf{m}(\mathbf{r})$ which explains why d_L^{SSW} does not vanish for the SSW UEG. In fact we see that d_L^{SSW} provides *the same* information as D_T^{SSW} , meaning, sq to some power. Adopting the convention that we obtain the characteristic parameters for the local xc energy using as few derivatives as possible $s(\mathbf{r})$ and $q(\mathbf{r})$ are determined through $D_T(\mathbf{r})$ and $d_T(\mathbf{r})$ by

$$s(\mathbf{r}) = \sqrt{\frac{D_T^2(\mathbf{r})}{D_T^2(\mathbf{r}) + m^4(\mathbf{r}) d_T(\mathbf{r})}}, \quad (16)$$

$$q(\mathbf{r}) = \sqrt{\frac{D_T^2(\mathbf{r}) + m^4(\mathbf{r}) d_T(\mathbf{r})}{m^4(\mathbf{r}) D_T(\mathbf{r})}}. \quad (17)$$

This completes the definition of the SSW functional Eq. (6) or equivalently the SGE to the LSDA Eq. (7).

By definition (c.f. Eq. (16)) the local $s(\mathbf{r})$ is between $[0, 1]$ in accordance with being the sine of an azimuthal angle. Furthermore we have the following hierarchy in the dependence of the SGE, Eq. (7), on the transverse gradients: i) If $D_T(\mathbf{r}) = 0$, the SGE correction is zero. ii) If $D_T(\mathbf{r}) \neq 0$ and $d_T(\mathbf{r}) = 0$, the SGE correction is obtained from a *planar* SSW ($s = 1$). iii) If both transverse gradients are non-zero the SGE correction is obtained from a general SSW.

We proceed by evaluating the xc magnetic field from the SSW functional,

$$\mathbf{B}_{xc}^{\text{SSW}}(\mathbf{r}) = -\frac{\delta E_{xc}[n, \mathbf{m}]}{\delta \mu_B \mathbf{m}(\mathbf{r})} = \mathbf{B}_{xc}^m + \mathbf{B}_{xc}^{D_T} + \mathbf{B}_{xc}^{d_T}, \quad (18)$$

where we split $\mathbf{B}_{xc}^{\text{SSW}}(\mathbf{r})$ into contributions coming from the dependence of $\varepsilon_{xc}^{\text{SSW}}$ on m , D_T and d_T , respectively. The explicit evaluation of $\mathbf{B}_{xc}^{\text{SSW}}(\mathbf{r})$ is straight-forward but rather lengthy. Here we will show the energetic content in the Kohn-Sham (KS) system, i.e. ,

$$E_{\mathbf{B}_{xc}}^{\text{KS}} = -\mu_B \int d^3r \mathbf{m}(\mathbf{r}) \cdot \mathbf{B}_{xc}(\mathbf{r}) = \int d^3r n(\mathbf{r}) (\partial_m \varepsilon_{xc}^{\text{SSW}}) m(\mathbf{r}) \quad (19)$$

$$+ 4 \int d^3r n(\mathbf{r}) (\partial_{D_T} \varepsilon_{xc}^{\text{SSW}}) D_T(\mathbf{r}) \quad (20)$$

$$+ 4 \int d^3r n(\mathbf{r}) (\partial_{d_T} \varepsilon_{xc}^{\text{SSW}}) d_T(\mathbf{r}). \quad (21)$$

The first term (Eq. (19)) is already present in the LSDA, whereas the other two terms (Eqs. (20),(21)) arise due to the inclusion of the SGE.

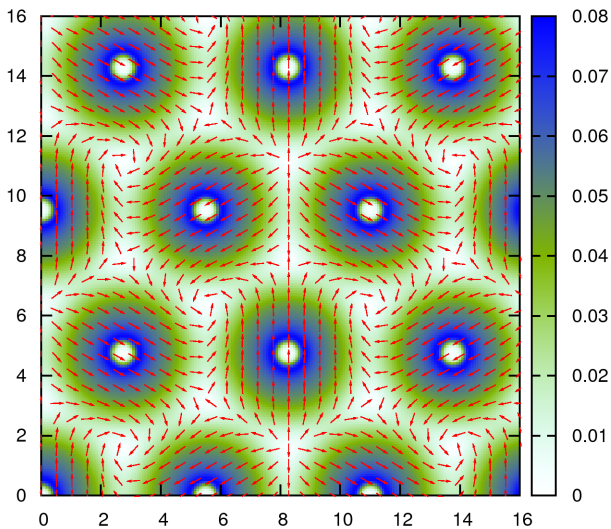


FIG. 1. (Color online). Magnitude (heat map) and direction (arrows) of $\mathbf{B}_{xc}(\mathbf{r})$ for the Cr mono-layer (LSDA).

The zero-torque theorem, Eq. (9), is fulfilled by construction, however the new terms in $\mathbf{B}_{xc}(\mathbf{r})$ are non-collinear w.r.t. $\mathbf{m}(\mathbf{r})$, i.e. , they provide a local torque

$$\mathbf{m}(\mathbf{r}) \times \mathbf{B}_{xc}(\mathbf{r}) \neq 0. \quad (22)$$

This local torque accounts for the fact that in SDFT the KS system *does not* reproduce the exact many-body currents (spin and charge) but only the exact many-body densities $n(\mathbf{r})$ and $\mathbf{m}(\mathbf{r})$ (review Ref. 11 for a detailed discussion). Comparing the equation of motion for $\mathbf{m}(\mathbf{r})$ in the many-body system and the KS system one obtains

$$\nabla \cdot \underline{\mathbf{J}}_{xc}(\mathbf{r}) = -2\mu_B \mathbf{m}(\mathbf{r}) \times \mathbf{B}_{xc}(\mathbf{r}), \quad (23)$$

where $\underline{\mathbf{J}}_{xc}(\mathbf{r})$ is the xc spin current defined as the difference between the many-body spin current $\underline{\mathbf{J}}(\mathbf{r})$ and the KS spin current $\underline{\mathbf{J}}_s(\mathbf{r})$. For the specific case of a vanishing *external* magnetic field (a case often studied in SDFT), we know that the many-body currents vanish and hence the transverse part of $\mathbf{B}_{xc}(\mathbf{r})$ determines the irrotational part of the KS spin current [12]. In other words, a system exhibiting spontaneous non-collinear magnetism is described by a KS system with non-vanishing irrotational spin current.

The final step for a practical implementation of the SSW functional is the determination of the SGE from the SSW UEG. We obtained $S_{xc}(n, m, s, q)$ using the random-phase approximation (RPA) for the SSW UEG. It is important to stress that we approximate the S_{xc} with the RPA and *not* $\varepsilon_{xc}^{\text{SSW}}$. In this way the SSW functional reduces to the usual LSDA and not to the RPA-LSDA, i.e. , the LSDA parametrized using the RPA xc energy of the UEG. From ~ 65000 data points in the four-dimensional domain of S_{xc} we constructed a polynomial fit for S_{xc} .

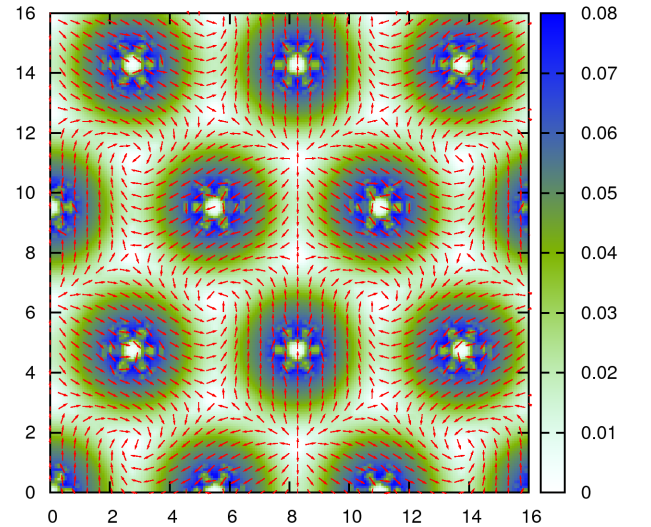


FIG. 2. (Color online). Same as FIG. 1 for the SSW functional. Note the intra-atomic non-collinearity of $\mathbf{B}_{xc}(\mathbf{r})$.

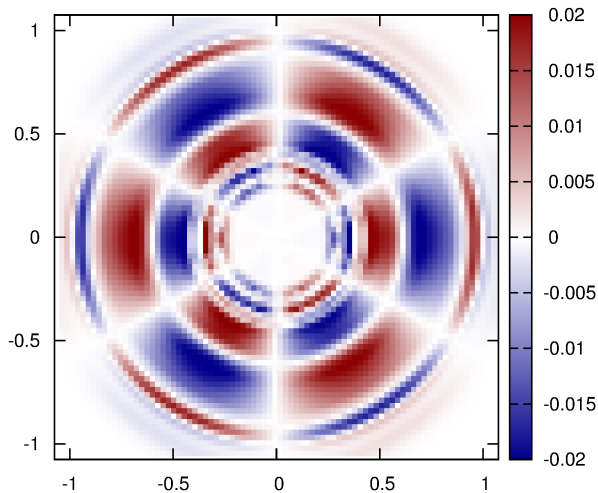


FIG. 3. (Color online). Heat map of the z -component of $\mathbf{m}(\mathbf{r}) \times \mathbf{B}_{xc}(\mathbf{r})$ around a Chromium atom in the mono-layer. A non-vanishing KS spin current for the non-collinear 120° -Néel state is implied (cf. Eq. (23)). Note the three-fold rotation symmetry inherited from the symmetry of the Chromium mono-layer. The zero-torque theorem (cf. (9)) may be inferred from the pattern of negative (blue) and positive (red) local torques.

As a proof-of-principle we implemented the SSW functional in the ELK code [13] in order to investigate the Chromium mono-layer in the 120° -Néel state. In FIGs. 1 and 2 we plot the magnitude and direction of \mathbf{B}_{xc} in order to illustrate the qualitative difference between the LSDA and the SSW functional. While the local spin magnetization $\mathbf{m}(\mathbf{r})$ are similar for the LSDA and the SSW functional, \mathbf{B}_{xc} obtained via the SGE exhibits much more structure compared to the LSDA \mathbf{B}_{xc} . As a result (cf. FIG. 3) the local torque does not vanish and a ground-state spin current is present in the KS system. Since the SSW functional is not restricted to small $q(\mathbf{r})$ it accounts for the intra-atomic non-collinearity.

In conclusion we proposed a novel functional for SDFT depending on the first and second order transverse gradients of $\mathbf{m}(\mathbf{r})$. We emphasize that this functional is formulated in terms of a SGE to the LSDA, which vanishes in the case of a collinear system. GGAs are also corrections to the LSDA, hence it is conceivable to employ the two corrections simultaneously. Since GGAs are constructed having collinear systems in mind, one may argue that the longitudinal gradients $D_L(\mathbf{r})$, $d_L(\mathbf{r})$ should enter in the GGA part. We are confident that the SGE will improve the ab-initio description of materials exhibiting a non-collinear magnetic structure, which recently came in focus due to the observation of a Skyrmion lattice in the itinerant-electron magnet MnSi [14].

While the corrections to the part of the $\mathbf{B}_{xc}(\mathbf{r})$ parallel to $\mathbf{m}(\mathbf{r})$ will adjust the energetics, the perpendicular part of $\mathbf{B}_{xc}(\mathbf{r})$ describes the xc corrections to the spin current,

which in turn is crucial for ab-initio spin dynamics. We hope that the functional presented in this letter will pave the road to a better description of domain wall motion and spin wave propagation from first principles in the framework of time-dependent SDFT.

In both aforementioned scenarios it is important to have a numerically accessible functional which, given currently available computing facilities, implies the use of semi-local functionals. We demonstrated that non-collinearity can be included by a generalization of the reference system employed in the LSDA and hence the numerical accessibility of the LSDA is retained in the SSW functional making it the ideal candidate for large scale quantum simulations.

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- [1] R. M. Dreizler and E. K. U. Gross, *Density Functional Theory* (Springer-Verlag, Berlin Heidelberg, 1990).
- [2] P. Hohenberg and W. Kohn, Phys. Rev. **136**, B864 (1964).
- [3] U. von Barth and L. Hedin, J. Phys. C **5**, 1629 (1972).
- [4] W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965).
- [5] D. Rappoport, N. R. M. Crawford, F. Furche, and K. Burke, “Approximate density functionals: Which should i choose?” in *Computational Inorganic and Bioinorganic Chemistry*, edited by E. I. Solomon, R. B. King, and R. A. Scott (Wiley, Chichester. Hoboken: Wiley, John & Sons, Inc., 2009).
- [6] J. Kübler, K.-H. Hock, J. Sticht, and A. Williams, J. Phys. F **18**, 469 (1988).
- [7] J. E. Peralta, G. E. Scuseria, and M. J. Frisch, Phys. Rev. B **75**, 125119 (2007); G. Scalmani and M. J. Frisch, J. Chem. Theory and Comput. **8**, 2193 (2012).
- [8] M. I. Katsnelson and V. P. Antropov, Phys. Rev. B **67**, 140406(R) (2003).
- [9] K. Capelle and B. L. Gyorffy, Europhys. Lett. **61**, 354 (2003).
- [10] A. W. Overhauser, Phys. Rev. **128**, 1437 (1962); G. F. Giuliani and G. Vignale, “Spin density wave and charge density wave hartree-fock states,” (Cambridge University Press, Cambridge, 2005) Chap. 2.6, pp. 90–101.
- [11] K. Capelle, G. Vignale, and B. L. Györfy, Phys. Rev. Lett. **78**, 206403 (2001).
- [12] Usually one refers to the irrotational part of currents as the longitudinal component. Since throughout the letter we are using longitudinal and transverse to describe orientations in spin space w.r.t. $\mathbf{m}(\mathbf{r})$, we refrain from using this nomenclature for the currents.
- [13] “The elk fp-lapw code,” <http://elk.sourceforge.net/>.
- [14] S. Mühlbauer, B. Binz, F. Jonietz, C. Pfleiderer, A. Rosch, A. Neubauer, R. Georgii, and P. Bni, Science **323**, 915 (2009).